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TITLE: Exchange Bias and Training Effect in Polycrystalline Antiferromagnetic/Ferromagnetic Bilayers

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Mat. Res. Soc. Symp. Proc. Vol. 746 © 2003 Materials Research Society Q7.6

Exchange Bias and Training Effect in Polycrystalline Antiferromagnetic/Ferromagnetic Bilayers

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ABSTRACT

Exchange bias and training effect are simulated for IrMn/NiFe bilayers. As a function of the thickness of the antiferromagnet the bias field shows a maximum for a thickness of 22 nm. For decreasing antiferromagnetic thickness the domain wall energy approaches zero. For large thicknesses the high anisotropy energy hinders switching of the antiferromagnetic grains resulting in weak bias. Starting from the field cooled state as initial configuration a bias field of about 8 mT is obtained assuming a antiferromagnetic layer thickness of 20 nm, a ferromagnetic layer thickness of 10 nm, and a grain size of 10 nm. The next hysteresis cycle shows a reduction of the bias field by about 65%. Exchange bias and training effect in fully compensated antiferromagnet/ferromagnet bilayers are explained with a simple micromagnetic model. The model assumes no defects except for grain boundaries, and coupling is due to spin flop at a perfect interface. The simulations show that a weak exchange interaction between randomly oriented antiferromagnetic grains and spin flop coupling at a perfectly compensated interface are sufficient to support exchange bias.

INTRODUCTION

The phenomena of exchange anisotropy and exchange bias, particularly, were discovered in the year 1956 by Meiklejohn and Bean [1] when studying Co particles surrounded with antiferromagnetic oxide (CoO). They found that the field required to switch the ferromagnet from the field cooled state into the reversed state is larger than that to rotate the ferromagnet back to its original direction. Since the introduction of the Giant Magnetic Resistance (GMR) head in magnetic recording [2] the bias effect has been used widely in modern technology. The pinned layer of a spin valve sensor is stabilized through coupling to an antiferromagnet. A common system used in GMR reading heads are IrMn/NiFe bilayers [3]. Despite the application of exhange bias in magnetic field sensors, the physical mechanisms that lead to the hysteresis shift are still a field of discussion. Various theories explain particular aspects of the bias effect [4]. Nevertheless many issues remain to be solved [5]. One of the most striking experimental facts is the presence of exchange bias at fully compensated antiferromagnetic (AF) interfaces [6,7] in which the net spin averaged over a microscopic length scale is zero. Intuitively, one might expect that for compensated interfaces the bias effect vanishes, as the spins pinning the ferromagnetic cancel. Therefore various models of exchange bias assume partly uncompensated interfaces [4].

In this paper we propose a mechanism for exchange bias at fully compensated interfaces. The numerical results obtained for IrMn/NiFe bilayers are compared with experimental data from the recent literature [8,9]. The simulations on a mesoscopic length scale show that a weak exchange interaction between randomly oriented AF grains and spin flop coupling at a perfectly compensated interface are sufficient to support exchange bias.

Originally, Koon [10] proposed a mechanism for exchange bias at fully compensated interfaces. Using an atomistic model Koon showed that a fully compensated antiferromagnetic interface will lead to a 90° coupling between the antiferromagnet and the ferromagnet. Indeed 90° coupling has been observed experimentally [6,7]. In Koon's model a weak canting of the antiferromagnetic spins close to the interface provide a small net magnetic moment parallel to the ferromagnetic magnetization direction. The antiferromagnet near the interface thus aligns perpendicular to the ferromagnet (spin flop coupling). Under the assumption that the antiferromagnetic spins are restricted to planes parallel to the interface, Koon was able to predict exchange bias. The loop shift can be attributed to partial domain walls wound up in the antiferromagnet. Allowing full three dimensional rotations of the antiferromagnetic spins, Schulthess and Butler [11] showed that the domain walls are unstable due to out of plane rotations of the antiferromagnetic spins. They conclude that spin flop coupling at compensated interfaces enhances the coercivity but does not lead to exchange bias. Stiles and McMichael [12] drew a similar conclusion introducing spin flop coupling in their model for polycrystalline ferromagnetic-antiferromagnetic bilayers.

Nowak and co-workers [13] proposed the so-called domain state model for exchange bias. In their model the antiferromagnet breaks up into magnetic domains due to domain wall pinning at random defects. The domains may carry a remanent surplus magnetization. This small net magnetic moment provides coupling across the interface. The authors find a bias shift for directions parallel to the antiferromagnetic anisotropy axis for spins in a single crystal lattice.

In our model we assume a perfectly compensated interface. The antiferromagnet is not a single crystal but a collection of grains with randomly oriented anisotropy direction. In contrast to the model of Stiles and McMichael [12] we assume weak exchange coupling between the grains. Using a finite element simulation with subgrain discretization, Suess and co-workers [14] showed that a perfectly compensated interface will lead to spin flop coupling which in turn causes exchange bias. Weak exchange interactions between the AF grains were essential: (1) They partly suppress out of plane rotations of the antiferromagnetic moments and (2) provide the wall energy between lateral antiferromagnetic domains. The simulation show that the reversal of the ferromagnet causes the formation of domains within the antiferromagnet: Some of the AF grains switch irreversibly when the ferromagnet reverses, whereas another part of the AF grains remain stable. After reversal of the ferromagnet the system stores energy in antiferromagnetic domain walls perpendicular to the interface, which in turn gives rise to the observed loop shift. The finite element approach showed that the magnetization configurations in the AF grains remain almost uniform during the reversal of the ferromagnet. Therefore, a granular model where the magnetization is actually uniform within the AF grains should yield very similar results but allows to simulate larger systems with the great advantage of avoiding possible finite size effects.

INTERACTING GRAIN MODEL

Let us consider a thin ferromagnetic film spin flop coupled to a polycrystalline antiferromagnet with randomly oriented easy axes. The magnetization configuration within the AF grains are assumed to be uniform. This is a good approximation for small grain sizes and low intergrain exchange coupling within the antiferromagnet. Due to the spin flop coupling the antiferromagnetic spins are not fully antiparallel near the interface. Since the deviation is small and relaxes very rapidly to the spin structure of the bulk we neglect the tilting of the spins. Thus, for the simplest case of two sublattices the magnetic state of each AF grain can be described by a single vector of one sublattice. The magnetization vector of the other sublattice points exactly antiparallel. This means that as long as the applied field is not larger than the antiferromagnetic exchange, as is the case in most experiments, magnetic surface and volume charges cancel in the antiferromagnet. Any remaining contributions to magnetostatic energy for individual magnetic sublattices in the antiferromagnet can be taken into account through the anisotropy constant, K_1. Shape effects for the ferromagnetic film are approximated with an in plane anisotropy energy in the ferromagnet.

The interacting grain model takes into account the intergrain exchange energy, the spin flop coupling energy [12,15], the anisotropy energy in the antiferromagnet, the demagnetization energy of the ferromagnet, and the Zeeman energy in an external field. The total energy of the ferromagnet (F) / antiferromagnet (AF) bilayer system per grain j is

$$
\begin{aligned}
E^j = \sum_{i=1}^{nN} & \left[-J_F S^2 n_F t_F l \left(\mathbf{u}_F^i \cdot \mathbf{u}_F^j \right) - J_{AF} S^2 n_{AF} t_{AF} l \left(\mathbf{u}_{AF}^i \cdot \mathbf{u}_{AF}^j \right) \right] \\
& - J_{AF\text{-}F} S^2 n_I l^2 \left(\mathbf{u}_{AF}^j \cdot \mathbf{u}_F^j \right)^2 - K_1 t_{AF} l^2 \left(\mathbf{k}_{AF}^j \cdot \mathbf{u}_{AF}^j \right)^2 \\
& - \frac{J_s^2}{\mu_0} t_F l^2 \left(\mathbf{k}_F^j \cdot \mathbf{u}_F^j \right)^2 - J_s t_F l^2 \left(\mathbf{H} \cdot \mathbf{u}_F^j \right).
\end{aligned} \tag{1}
$$

The sum over i is carried out only over the nearest neighbor grains in the antiferromagnet and ferromagnet, respectively. Here $\mathbf{u}$ is the unit of the magnetization, J is the exchange integral, S is the average total spin quantum number, $\mathbf{k}$ is the a unit vector parallel to the uniaxial anisotropy axis, t is the layer thickness, l is the grain size, $\mathbf{H}$ is the external field, and J_s is the spontaneous magnetic polarization of the ferromagnet. The indices AF, F, and AF-F (or I) denote the antiferromagnet, the ferromagnet, and the antiferromagnetic/ferromagnetic interface, respectively. For simple cubic lattices with lattice constant a we find for the number of spins per unit area: $n_F = n_{AF} = n_I = 1/a^2$ and for the spontaneous polarization $J_s = \mu_0 g \mu_B S/a^3$. Here μ_B is the Bohr magneton and g is the Landé factor.

Calculations are performed by first choosing the magnetocrystalline anisotropy axes of the AF grains randomly in space and then initializing the system by simulating field cooling. Afterwards, the evolution of the magnetization configuration with changing external field is investigated. A Metropolis Monte Carlo algorithm similar to that introduced by Hinzke and Nowak [16] is used to simulate field cooling. The hysteresis loops are calculated quasistatically: An equilibrium configuration is obtained by the numerical integration of the Landau-Lifshitz Gilbert equation at value of the external field. The field step was 2 mT.

RESULTS AND DISCUSSION

Experimentally, the exchange bias field is inversely proportional to ferromagnetic layer thickness, t_F. This relation breaks down for small t_F [5]. The thickness of the antiferromagnetic film has to exceed a certain critical thickness to find exchange bias. H_{eb} decreases abruptly for small t_{AF}. For large antiferromagnetic thickness two different effects are found. In most systems the bias field remains constant for $t_{AF} > 20$ nm. However, in some systems the thickness of H_{eb} is reduced for large t_{AF}. In addition in some systems, as t_{AF} is reduced, $H_{eb}(t_{AF})$ shows a pronounced peak before the main decrease [5]. Van Driel and co-workers [9] measured the dependence of H_{eb} on antiferromagnetic layer for textured and randomly oriented IrMn/Ni bilayers. They found that the maximum of the peak is shifted towards smaller t_{AF} in the <111> textured film.

In the following we present the results for the thickness dependence of the exchange bias field for IrMn/NiFe bilayers. In addition we compare the computed magnetization structure in the ferromagnet with magnetic images obtained by transmission electron microscopy [8]. IrMn for exchange biased bilayer systems is used in the disordered fcc (γ) phase. The average spins on each (002) plane are aligned parallel along the c-axis with alternating signs on neighboring (002) planes [4]. In terms of magnetic anisotropies, a <111> texture corresponds to an average angle of 54.74° between the easy axes and the interface normal. We calculated $H_{eb}(t_{AF})$ for randomly oriented IrMn grains and for <111> textured films assuming a Gaussian distribution of the magnetocrystalline anisotropy direction with a standard deviation of 20°. The material parameters used for the simulations were $J_F = 0.43$ meV, $J_{AF} = 0.023$ meV, $J_{AF\text{-}F} = 0.043$ meV, $K_1 = 10^5$ J/m³, $l = 10$ nm, and $J_s = 1$ T.

Figure 1 gives the calculated dependence of the bias field and of the coercivity on the ferromagnetic layer thickness and shows the influence of texture on $H_{eb}(t_{AF})$. The bias field is proportional to $1/t_F$ as long as $t_F \geq 10$nm. The bias field as a function of t_{AF} shows a maximum. The maximum bias field of about 9mT is reached for t_{AF} between 20 nm and 30 nm for the randomly oriented bilayer. The maximum is shifted towards 15 nm for the <111> textured IrMn/NiFe bilayer. Detailed investigations showed that there is a clear correlation between the number of switched AF grains and the bias field. As the ferromagnet is reversed a small fraction of the AF grains switches irreversible. The large antiferromagnetic domains which a formed during field cooling break up into smaller domains. The reversed state stores some additional domain wall energy which in turn leads to exchange bias. The wall energy depends on the pattern of switched AF grains. The bias field was found to be proportional to the ratio C/C_{max}, where C is the circumference of the pattern of switched AF grains and C_{max} is the maximum possible circumference. The relation $H_{eb} \propto (C/C_{max})\, t_{AF}$ holds for the entire thickness range which confirms that exhange bias is associated with the domain wall energy stored in the lateral AF domains.

King and co-workers [8] observed 360° wall loops during the reversal of the ferromagnet in IrMn/NiFe bilayers. Such loops, once formed, were remarkably stable and remained up to fields of about 300 Oe. Beyond this, the ferromagnetic film appeared saturated.

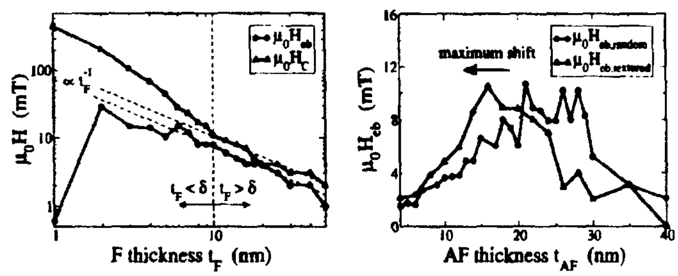

Figure 1. Calculated thickness dependence of the bias field of an IrMn/NiFe bilayer. Left hand side: H_{eb} and H_c as a function of the ferromagnetic layer thickness, $t_{AF} = 20$ nm. Right hand side: H_{eb} as a function of the antiferromagnetic layer thickness, $t_F = 10$ nm for randomly oriented and textured IrMn grains.

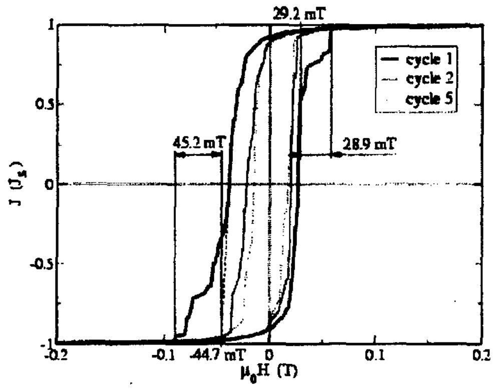

Figure 2. Calculated hysteresis loops for a $J_F = 0.129$ meV, $J_{AF} = 0.023$ meV, $J_{AF\text{-}F} = 0.043$ meV, $K_1 = 10^5$ J/m³, $l = 10$ nm, $t_F = 10$ nm, $t_{AF} = 20$ nm and $J_s = 1$ T. The knee in the hysteresis loop is due to the formation and annihilation of a 360° domain wall loop.

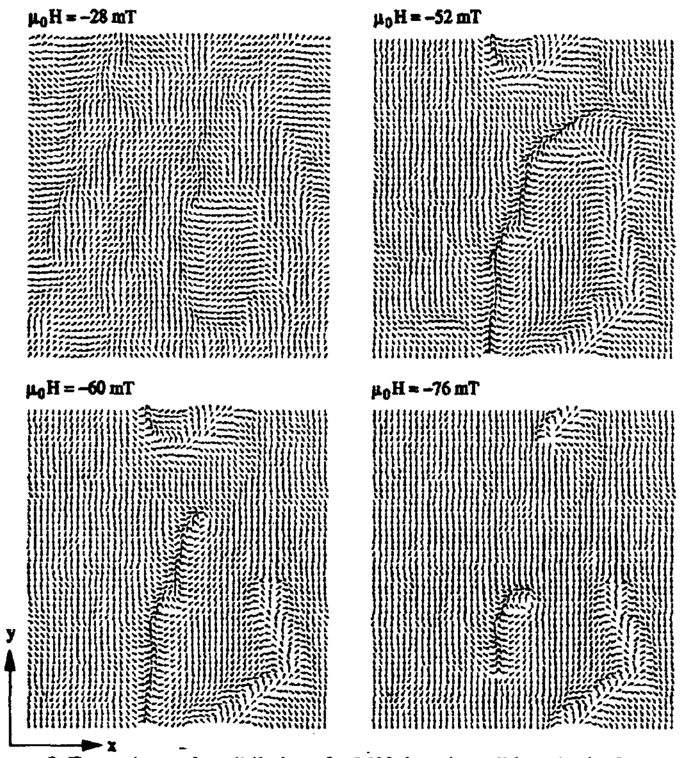

Figure 3. Formation and annihilation of a 360° domain wall loop in the ferromagnet.

To ensure their annihilation a substantially high external field had to be applied. Repetition of the hysteresis cycle showed a similar behavior, but the locations of theses loops tended to vary.

In our simulations stable 360° wall loops or lines appeared primarily for $J_F = 0.129$ meV. Figure 2 shows the calculated hysteresis loops. At $\mu_0 H = 40$ mT domain walls move together and, rather than annihilating, form a 360° wall loop as shown in figure 3. This configuration is stable due to the pinning effect of the antiferromagnetic layer, leading to a distinct knee in the hysteresis curve.

In addition figure 2 shows a training effect, the decrease of the loop shift and of the coercivity with increasing number of hysteresis cycles. When the ferromagnet is switched back the antiferromagnetic domain structure that was formed after field cooling is not fully recovered. Each cycle through the magnetization loop brings the antiferromagnet closer to a type of dynamic equilibrium in which the coercive field no longer changes with each additional cycle and the loop area remains constant. In our simulations, this equilibrium appeared after about four cycles.

ACKNOWLEDGEMENTS

The authors thank R. L. Stamps, J. V. Kim (University of Western Australia) and J. N. Chapman (University of Glasgow) for helpful discussion.

This work was supported by the Austrian Science Fund (Y-132 PHY).

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